

Unusual Metallic Conductivity of Underdoped and Optimally Doped Cuprates: Evidence for Competing Fermi-Liquid and Pairing Pseudogap Effects

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We propose a possible scenario for the new metallic conductivity of underdoped and optimally doped cuprates. Charge carriers are assumed to be large polarons which form a Fermi-liquid and Cooper-like pairs below a crossover temperature T^* . We use the Boltzmann equation to calculate the conductivity of self-trapped carriers and the resistivity ρ as a function of temperature and doping for different cuprates. We show that various anomalies in $\rho(T)$ below T^* are caused by the competing Fermi-liquid and BCS-like precursor pairing effects. Our results for ρ fit well with existing experiments and characterize high- T_c cuprates with an intermediate-coupling.

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Understanding the normal-state charge transport properties of the high- T_c cuprates remains one of the central issues in condensed matter physics [1, 2, 3, 4]. Many experimental studies [5, 6, 7, 8] have shown that in the underdoped and optimally doped cuprates, the resistivity ρ shows anomalous temperature dependences as well as a complicated doping dependence. There is much evidence for the crossover regime at some temperature $T^* > T_c$ in these materials and ρ shows a T -linear dependence above T^* . However, for the underdoped cuprates $\rho(T)$ starts to deviate downward from the T -linear behavior below T^* . In contrast, in the optimally doped cuprates, $\rho(T)$ is roughly linear below T^* . Sometimes the anomalous resistive transitions (i.e., a sharp drop and small jump in $\rho(T)$) are observed at T^* in some cuprates (see, Refs. [9, 10]). The anomalies in $\rho(T)$ at $T \leq T^*$ are thought to arise from a pseudogap (PG) state which has been observed by NMR, ARPES and other experiments [11, 12, 13]. The origin of the PG is still controversial. A number of theoretical models have been proposed, which rely on different non-phononic mechanisms of pairing (including precursor superconducting (SC) fluctuations) [14, 15]. On the other hand, there is convincing experimental evidence for a strong electron-phonon interaction in the cuprates [13, 16, 17]. One possible scenario involving electron-phonon interactions is based on the BCS-like non-SC (i.e., precursor) pairing model [18]. It was postulated in this model that the formation of the non-SC Cooper-like polaron pairs is quite possible in the normal state, while their condensation into a superfluid Bose liquid state would occur only at T_c . Further, it was argued that the pairing PG and true SC gap have different origins and coexist below T_c . Recent experimental results [19, 20] support such a picture and put much more severe constraints on theories of precursor SC fluctuations. The opening of the pairing PG in the normal state of the cuprates should affect their transport properties. But the effect of the BCS-like non-SC gap (or PG) on the charge transport in cuprates has not previously been studied. Another open question is the

relevance of a Fermi-liquid picture to the normal state of the underdoped and optimally doped cuprates [4, 13].

So far, the T -linear resistivity in the cuprates have been explained in terms of non-Fermi-liquid (including the RVB [21], marginal Fermi-liquid [22] and bipolaronic [23]) models and different Fermi-liquid scenarios (see Ref. [3]). However, rather little is known theoretically [3, 24] about the above anomalies in $\rho(T)$ and how the electron-phonon coupling, Fermi-liquid and BCS-like precursor pairing correlations influence on the normal-state charge transport properties of high- T_c cuprates.

In this letter, we address these questions and propose a possible scenario for the new metallic conductivity of underdoped and optimally doped cuprates. A key is that the doped carriers in these materials above T^* are the non-interacting large polarons, while below T^* they form a polaronic Fermi-liquid and Cooper-like pairs. These large polarons are scattered by acoustic phonons. We argue that the T -linear resistivity in underdoped and optimally doped cuprates above T^* is due to the carrier-phonon scattering. We then show how the competing Fermi-liquid and BCS-like precursor pairing correlations lead to the characteristic deviations from the T -linear behavior in $\rho(T)$ below T^* and the distinctly different resistive transitions at T^* , which are very similar to the existing experimental data on cuprates. We find that the Fermi-liquid parameter F_1^s decreases as the BCS-like pairing PG or T^* grows towards underdoped regime.

Relevant charge carriers in doped cuprates. — The underdoped cuprates are the charge-transfer (CT)-type Mott insulators. Upon doping the oxygen valence band of the cuprates is occupied by holes. These charge carriers being placed in a polar crystal will interact with the acoustic and optical phonons, and the ground states of the doped carriers interacting with lattice vibrations are their self-trapped (polaronic) states lying in the CT gap of cuprates. Theoretical [25] and experimental [26] studies show that the relevant charge carriers in doped cuprates are polaronic quasiparticles and the electron-phonon interaction is responsible for the enhanced polaron mass

$m_p = 2 - 2.5m_e$ [26, 27] (where m_e is the free electron mass).

Large-polaron transport above T^ .* — As the doping x (e.g., in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$) is increased towards the underdoped level, the hole-doped cuprates evolve towards intermediate electron-phonon coupling regime and enter the strange metallic state. We assume that the doped carriers in the metallic state of high- T_c cuprates are degenerate large polarons and form a non-interacting Fermi-gas above T^* . We calculate the conductivity of these polarons using the Boltzmann equation in the relaxation time approximation. The Fermi energy of large polarons $\varepsilon_F = (\hbar^2/2m_p)(3\pi^2n_p)^{2/3}$ (where n_p is the concentration of large polarons) is of order 0.1 eV or greater and the condition $\varepsilon_F \gg k_B T$ is satisfied even well above T^* . We argue that the scattering of large polarons by acoustic phonons determines their transport relaxation rate which depends on the polaron energy ε and is linear in temperature [28]:

$$\frac{1}{\tau(\varepsilon)} = \frac{E_d^2(2m_p)^{3/2}\varepsilon^{1/2}k_B T}{\pi\rho_M\hbar^4v_s^2}, \quad (1)$$

where E_d is the deformation potential, ρ_M is the density of the materials, v_s is the sound velocity.

The conductivity σ is then calculated as

$$\sigma = -\frac{2n_p e^2}{3m_p} \cdot \frac{\int \varepsilon^{3/2} \tau(\varepsilon) (\partial f_0 / \partial \varepsilon) d\varepsilon}{\int \varepsilon^{1/2} f_0(\varepsilon) d\varepsilon}, \quad (2)$$

where $f_0(\varepsilon) = [1 + \exp(\varepsilon/k_B T)]^{-1}$ is the Fermi distribution function. The integrals in Eq. (2) can be evaluated using the standard approximations — $\partial f_0 / \partial \varepsilon = \delta(\varepsilon - \varepsilon_F)$, $f_0(\varepsilon < \varepsilon_F) = 1$ and $f_0(\varepsilon > \varepsilon_F) = 0$. Hence, for $T > T^*$ the conductivity is given by

$$\sigma(T) = \frac{2\pi\hbar^4 n_p e^2 \rho_M v_s^2}{E_d^2 (2m_p)^{5/2} \varepsilon_F^{1/2} k_B T}. \quad (3)$$

Fermi-liquid and BCS-like precursor pairing correlations below T^ .* — We now turn to the Fermi-liquid and BCS-like precursor pairing scenarios below T^* . We now make the key assumption that the large polarons begin to form an interacting Fermi-liquid and non-SC Cooper-like polaron pairs below T^* . In this case, in addition to the contribution of the electron-phonon interaction to the carrier effective mass, there is a contribution from the carrier-carrier interaction. The polaron mass m_p is then altered to $m_p^* = m_p(1 + \frac{1}{3}F_1^s)$, where F_1^s is the Landau parameter. In principle, the BCS-like pairing of carriers may occur, depending on the electron-phonon coupling strength, not only at T_c but also far above T_c [18]. In the weak-coupling regime, the pure dynamic-phonon-mediated BCS pairing occurs at T_c . While in the strong-coupling limit, the static-phonon-mediated non-BCS pairing occurs in the real

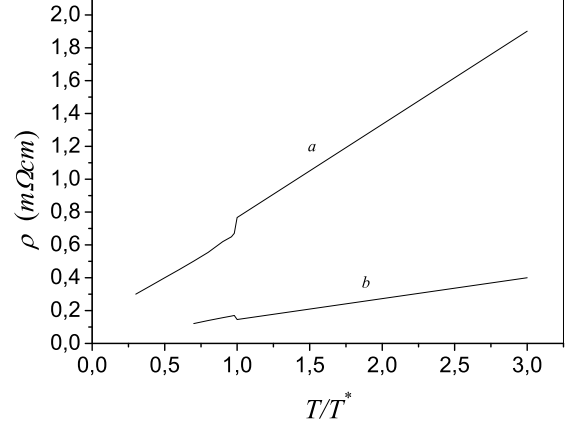


FIG. 1: Temperature dependence of ρ calculated for an underdoped (curve a) and optimally doped (curve b) system exhibiting distinctly different Fermi-liquid and PG behaviors.

space. Hence, the combined static- and dynamic-phonon-mediated BCS-like pairing at some temperature $T^* > T_c$ should occur in the intermediate-coupling regime.

A generalized BCS-like formalism, applied to self-trapped quasiparticles with a well defined density of states $D(\varepsilon)$, leads to the following gap (or PG) equation:

$$\Delta_F(k, T) = - \sum_{k'} V_{kk'} \frac{\Delta_F(k', T)}{2E(k', T)} \tanh \frac{E(k', T)}{2k_B T}, \quad (4)$$

where $E(k, T) = \sqrt{\varepsilon^2(k) + \Delta_F^2(k, T)}$, $V_{kk'}$ is the pair interaction potential between polarons approximated as [18]

$$V_{kk'} = \begin{cases} V_C - V_A, & 0 \leq \varepsilon(k), \varepsilon(k') \leq \varepsilon_A, \\ V_C & \varepsilon_A \leq \varepsilon(k), \varepsilon(k') \leq \varepsilon_C, \\ 0 & \text{otherwise,} \end{cases} \quad (5)$$

with the cut-off energies $\varepsilon_A = E_{bB} + \hbar\omega$ and $\varepsilon_C \gg \varepsilon_A$ for the attractive V_A and repulsive V_C parts of $V_{kk'}$, respectively, E_{bB} is the binding energy of a large bipolaron (real space pairs), ω is a characteristic phonon frequency. The solution of Eq. (4), which is obtained numerically using the model potential (5), gives $\Delta_F(T)$. The PG temperature T^* corresponding to $\Delta_F(T^*) = 0$ is given by $1.76k_B T^* = \Delta_F(0) = \varepsilon_A / \sinh(1/\lambda_{BCS})$, where $\lambda_{BCS} = D(0)\tilde{V}$ is the BCS-like coupling constant, $\tilde{V} = V_A - V_C/[1 + D(0)V_C \ln(\varepsilon_C/\varepsilon_A)]$ is the effective pairing potential. Below T^* , almost all polarons, which take part in conduction, have the energies smaller than ε_A and Fermi distribution function has the form $f_0(\varepsilon) = [1 + \exp(\sqrt{\varepsilon^2 + \Delta_F^2}/k_B T)]^{-1}$. The contribution of polarons with $\varepsilon > \varepsilon_A$ to the conductivity is negligible and can be ignored. Thus, the conductivity below T^* is

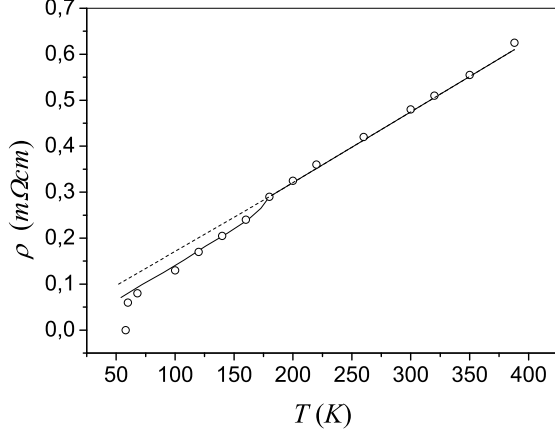


FIG. 2: The calculated temperature dependence of ρ (solid line) compared with experimental data on $\text{YBa}_2\text{Cu}_3\text{O}_{6.61}$ (taken from Ref. [5]) (open circles)

given by

$$\sigma(T) = \frac{A \cdot \int_0^{\varepsilon_A} \left\{ f_0(\varepsilon)[1 - f_0(\varepsilon)] / \sqrt{\varepsilon^2 + \Delta_F^2} \right\} \varepsilon^2 d\varepsilon}{(k_B T)^2 \int_0^{\varepsilon_A} f_0(\varepsilon) \varepsilon^{1/2} d\varepsilon}, \quad (6)$$

where $A = 4\pi\hbar^4 n_p e^2 \rho_M v_s^2 / 3E_d^2 [2m_p(1 + \frac{1}{3}F_1^s)]^{5/2}$.

Competing Fermi-liquid and pairing pseudogap effects.

— We use the solution of Eq. (4) to calculate $\sigma(T < T^*)$ by numerical integrating Eq. (6). Here and below we use the fixed value $\varepsilon_A = 0.08\text{eV}$. Since, E_{bB} increases with increasing the electron-phonon interaction strength, while ω decreases due to the phonon softening. Hence, ε_A is nearly independent of doping. The Fermi energy for undoped cuprates is about $E_F = 7\text{ eV}$ [29] and E_d is estimated as $E_d = (2/3)E_F$. The values of ρ_M and v_s lie in the ranges $\rho_M \simeq 6 - 7\text{ g/cm}^3$ and $v_s \simeq (5 - 7) \cdot 10^5\text{ cm/s}$ [1, 30]. Here we take $\rho_M = 6\text{ g/cm}^3$ and $v_s = 5 \cdot 10^5\text{ cm/s}$. To illustrate the competing Fermi-liquid and pairing PG effects on the resistivity $\rho(T) = \rho_0 + 1/\sigma(T)$ (where ρ_0 is the residual resistivity), we show in Fig. 1 results of our calculations for an underdoped (curve *a*) and optimally doped (curve *b*) system obtained using the parameters $m_p = 2.2m_e$, $F_1^s = 0.15$, $\lambda_{BCS} = 0.67$, $T^* = 250\text{K}$, $n_p = 0.46 \cdot 10^{21}\text{ cm}^{-3}$, $\rho_0 = 0, 2\text{ m}\Omega\text{cm}$ and $m_p = 1.7m_e$, $F_1^s = 1.8$, $\lambda_{BCS} = 0.49$, $T^* = 140\text{K}$, $n_p = 0.85 \cdot 10^{21}\text{ cm}^{-3}$, $\rho_0 = 0.02\text{ m}\Omega\text{cm}$, respectively. We find that the anomalies (i.e., a sharp drop and small jump) in $\rho(T)$ reflect the competing Fermi-liquid and PG effects below T^* . These anomalies in $\rho(T)$ are similar to the resistive transitions observed above T_c in some cuprates [9, 10]. The Fermi-liquid effect is expected to disappear in the heavily underdoped regime.

Comparison with existing experiments. — For

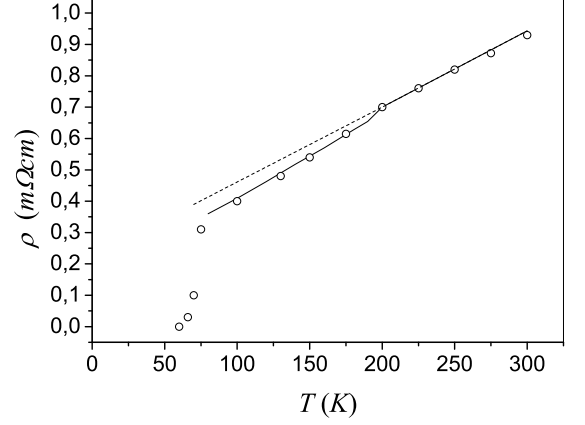


FIG. 3: The calculated temperature dependence of ρ (solid line) compared with experimental data on $\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_8$ (taken from Ref. [7]) (open circles)

TABLE I: Fitting parameters for underdoped and optimally doped cases. The values of T^* are taken from Refs. [5-8]

Sample	$n_p, 10^{21}\text{ cm}^{-3}$	F_1^s	λ_{BCS}	T^*, K	$\rho_0 (\text{m}\Omega\text{cm})$
$\text{YBa}_2\text{Cu}_3\text{O}_{6.1}$	0.52	0.60	0.557	180	0.020
$\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_8$	0.50	0.57	0.585	200	0.214
$\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$	0.50	0.54	0.585	200	0.210
$\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$	0.80	1.44	0.508	150	0.017

the comparison with existing experimental data we also present our results for T -dependent resistivity in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.1}$, $\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_8$, $\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$ and optimally doped $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ with the appropriate sets of fitting parameters. Some relevant parameters were: (i) $m_p = 2.3m_e$, $\rho_M = 6.4\text{ g/cm}^3$ and $v_s = 6 \cdot 10^5\text{ cm/s}$ for $\text{YBa}_2\text{Cu}_3\text{O}_{6.1}$; (ii) $m_p = 2.2m_e$, $\rho_M = 6\text{ g/cm}^3$ and $v_s = 4.7 \cdot 10^5\text{ cm/s}$ for $\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_8$; (iii) $m_p = 2.2m_e$, $\rho_M = 6.1\text{ g/cm}^3$ and $v_s = 5 \cdot 10^5\text{ cm/s}$ for $\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$ and (iv) $m_p = 1.8m_e$, $\rho_M = 6.9\text{ g/cm}^3$ and $v_s = 5.5 \cdot 10^5\text{ cm/s}$ for $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. Other fitting parameters are presented in Table 1. The best fits are obtained (see Figs. 2-5) if the combined Fermi-liquid and PG effects are taken into account. We believe that the present theory describes well both the T -linear behavior of $\rho(T)$ above T^* and the distinctly different deviations from the T -linear behavior in $\rho(T)$ below T^* . One can see that the gradual evolution of $\rho(T)$ with doping from a pronounced non-linear behavior in the underdoped regime to the nearly T -linear behavior at some optimal doping is associated with the competition between Fermi-liquid and PG effects. For larger values of the PG Δ_F , the Fermi-liquid parameter F_1^s will be smaller.

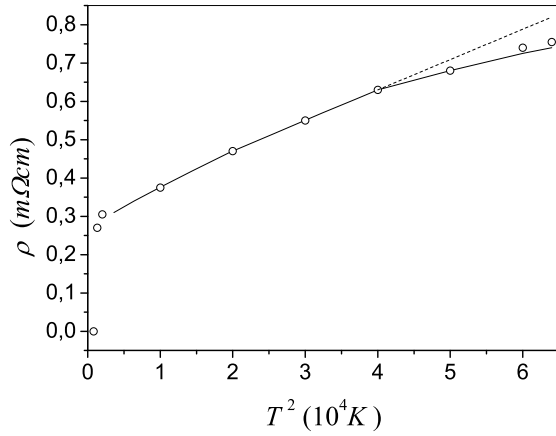


FIG. 4: The calculated temperature dependence of ρ (solid line) compared with experimental data on $\text{La}_{1.92}\text{Sr}_{0.08}\text{CuO}_4$ (taken from Ref. [8]) (open circles)

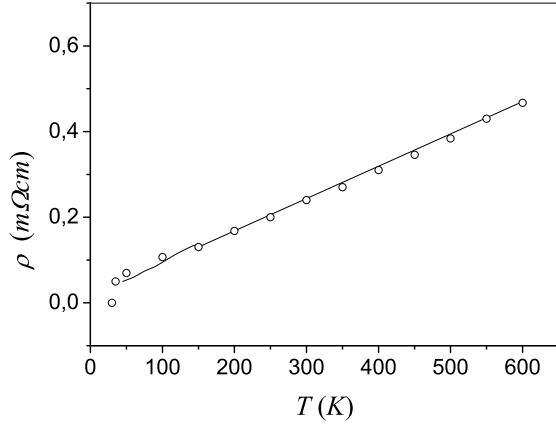


FIG. 5: The calculated temperature dependence of ρ (solid line) compared with experimental data on $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ (taken from Ref. [6]) (open circles)

In conclusion, we have studied the unusual metallic conductivity of self-trapped carriers (large polarons) in the normal state of underdoped and optimally doped cuprates. These quasiparticles are assumed to form a noninteracting polaronic gas above T^* and an interacting polaronic Fermi-liquid below T^* . We argue that the linear T -resistivity in underdoped and optimally doped cuprates could actually be due to carrier-phonon scattering. We have found that the distinctly different anomalies (e.g., a sharp drop and small upturn, a gradual downward deviation from the T -linear behavior, vanishing nonlinearity) in $\rho(T)$ occurring in these materials at T^* or below T^* are caused by the competing polaronic

Fermi-liquid and pairing PG effects. The proposed theory gives a good quantitative description of the systematic evolution of $\rho(T)$ with doping observed in cuprates.

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